Simulations of Granular Flow in Pebble-Bed Nuclear Reactors

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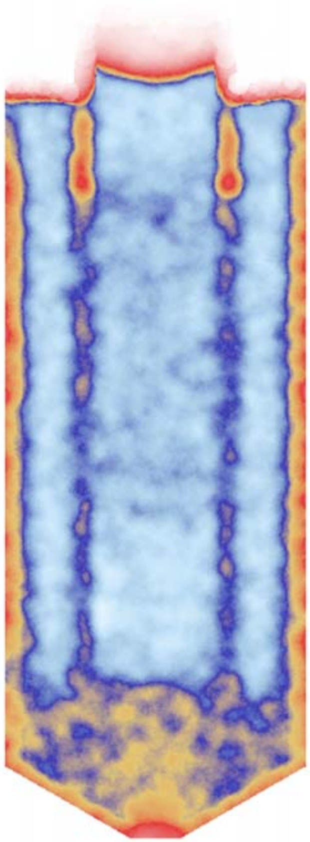
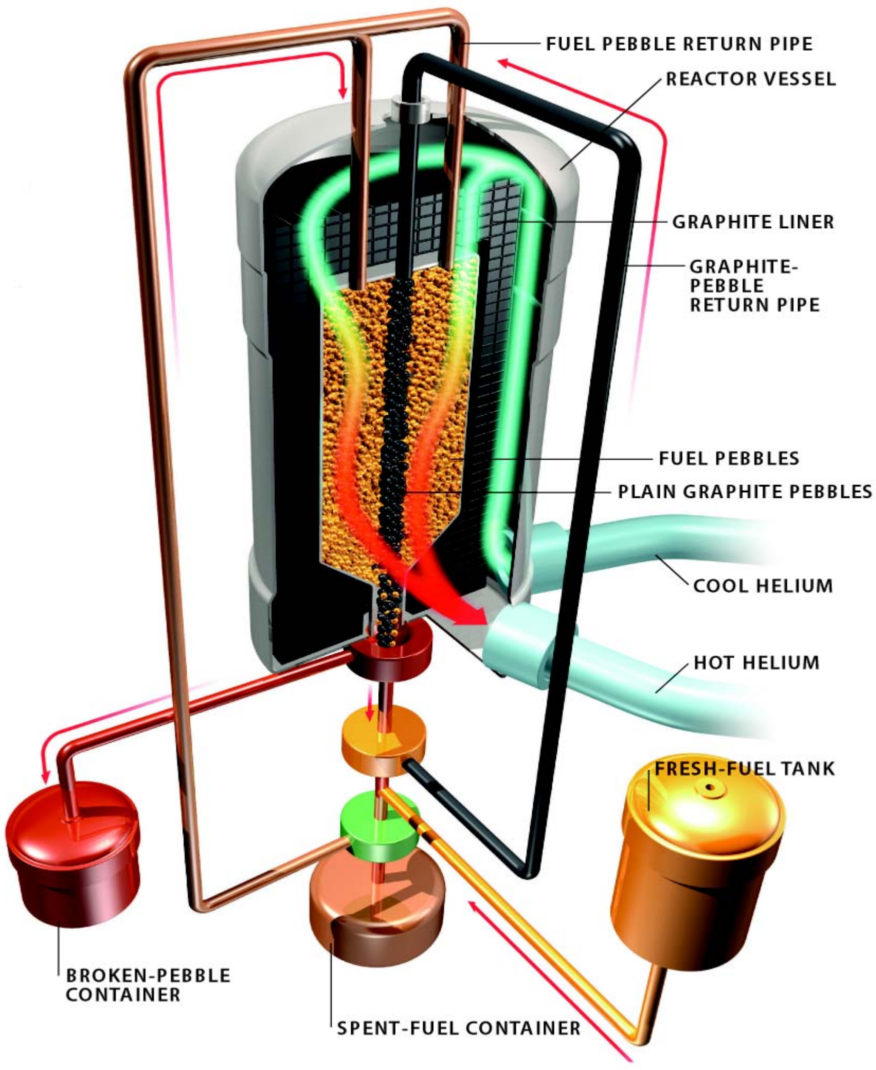
QuickTime™ and a
Cinepak decompressor
are needed to see this picture.



MIT/INL Modular Pebble-Bed Reactor

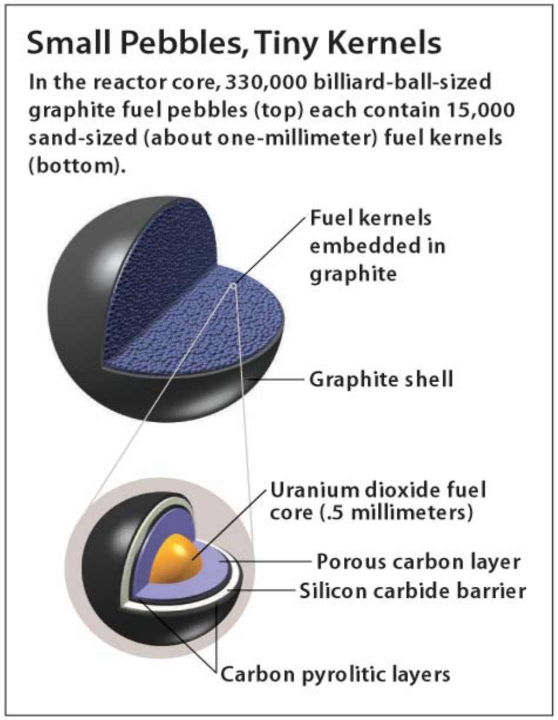
http://web.mit.edu/pebble-bed



MIT Technology Review (2001)

Reactor Core :

- D = 3.5 m
- H = 8-10m
- 100,000 pebbles
- d = 6 cm
- Q =1 pebble/min



Experiments and Simulations

MIT Dry Fluids Lab
http://math.mit.edu/dryfluids

Half-Reactor Model
("coke bottle")
Kadak & Bazant (2004)
Plastic, metal, or glass beads

3d Full-Scale MPBR
DEM Simulations
Rycroft, Bazant, Grest, Landry (2005)
Rycroft, Grest, Landry, Bazant (2006)
Frictional, visco-elastic spheres

QuickTime™ and a
Cinepak decompressor
are needed to see this picture.

Quasi-2d Silo Experiments
Choi et al., Phys. Rev. Lett. (2003)
Choi et al., J. Phys. Condensed Matter (2005)
Digital-video particle tracking

Discrete-Element Simulations of MPBR

- Sandia Lab parallel code (Gary Grest)
- Spheres with Hertzian, viscoelastic contacts
- normal force

$$\mathbf{F}_n = \sqrt{\delta/d}\left(k_n \delta \mathbf{n} - \frac{\gamma_n \mathbf{v}_n}{2}\right) \qquad \delta = d - |\mathbf{r}|$$

- tangential force

$$\mathbf{F}_t = \sqrt{\delta/d}\left(-k_t \Delta \mathbf{s}_t - \frac{\gamma_t \mathbf{v}_t}{2}\right)$$

- Coulomb yield criterion

$$|\mathbf{F}_t| \leq \mu |\mathbf{F}_n|$$

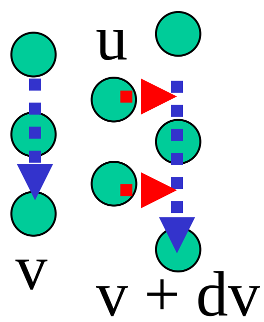
- N=440,000 pebbles draining once takes 13 hours on 60 processors on Sandia's Intel Xenon and generates 20 Gb of data

QuickTime™ and a
Cinepak decompressor
are needed to see this picture.

Velocity Profile in MPBR

"Kinematic Model"

Mullins (1972), Nedderman & Tuzun (1979).

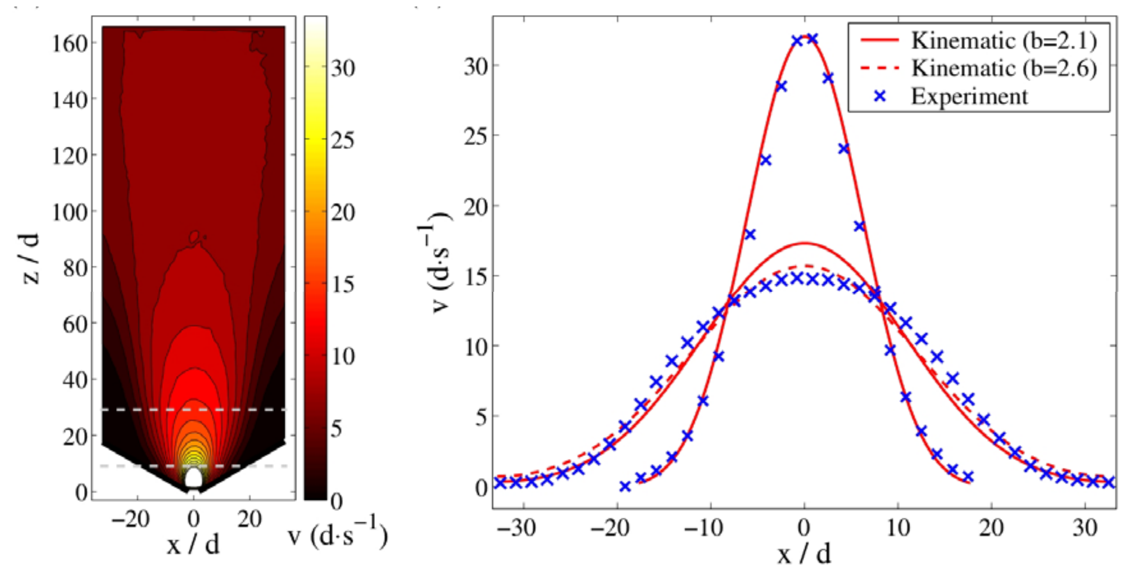


$$u = b\,\frac{\partial v}{\partial x}\;,\qquad \frac{\partial v}{\partial z} = b\,\frac{\partial^2 v}{\partial x^2}$$

- Good fit to experiments & DEM simulations in the bottom funnel; parabolic flow, corner stagnation

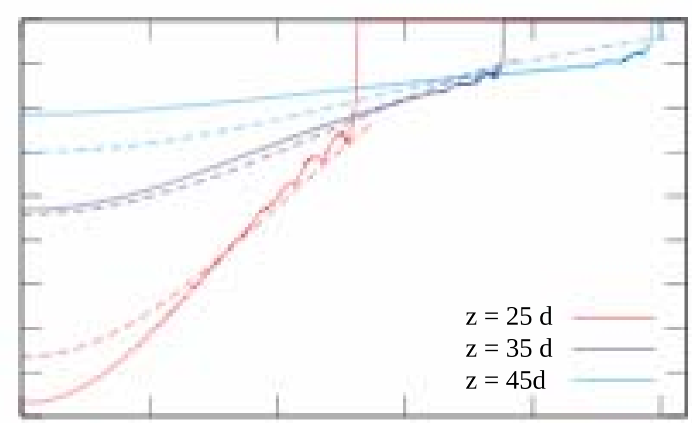
- Upper region is more like a plug

QUASI 2D EXPERIMENT: Choi, Kudrolli & Bazant (2005).



3D DEM SIMULATION: Rycroft, Grest, Landry, Bazant (2005).

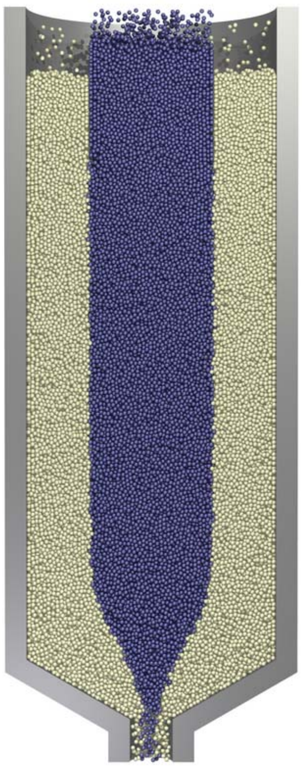
QuickTime™ and a Cinepak decompressor are needed to see this picture.



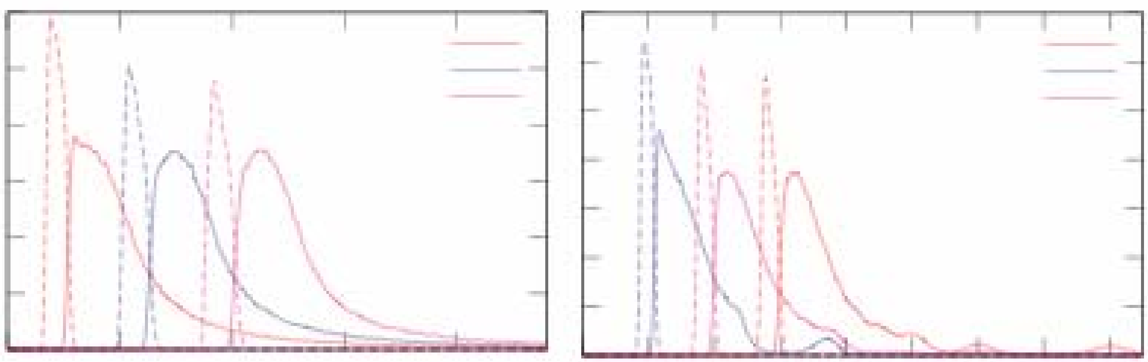
Pebble Mixing and Residence Times

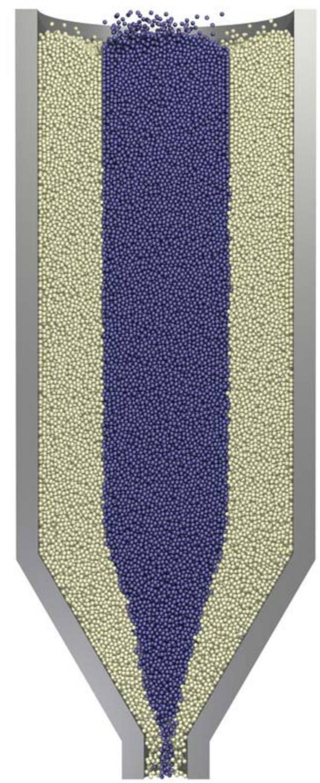
Horizontal diffusion
- very small (< d)
- stable moderator column
- no mixing with fuel pebbles (with upper guide ring)

Residence time distributions
- fat tailed, due to stagnation in corners
- better: more narrow funnel
- best: parabolic funnel



Residence times: moderator (dashed), fuel (solid)

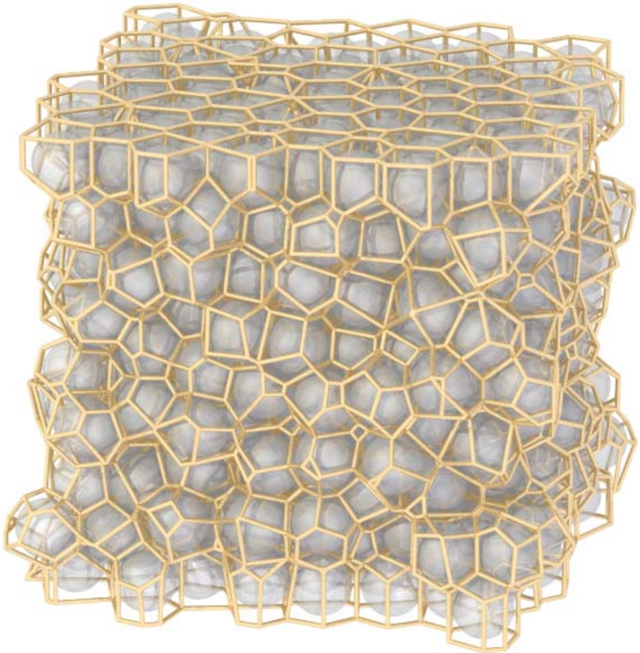




CONCLUSION:
The dynamic central column
is feasible with a guide ring.

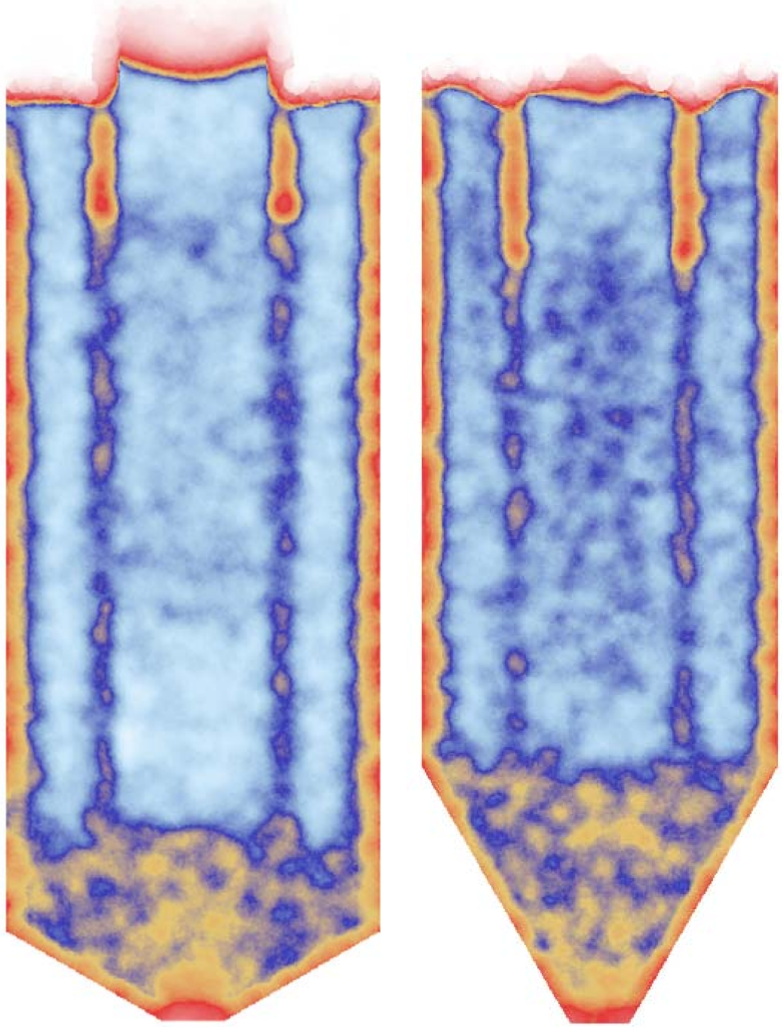
Core Porosity and Gas Permeability

Voronoi tesselation of a *flowing* packing



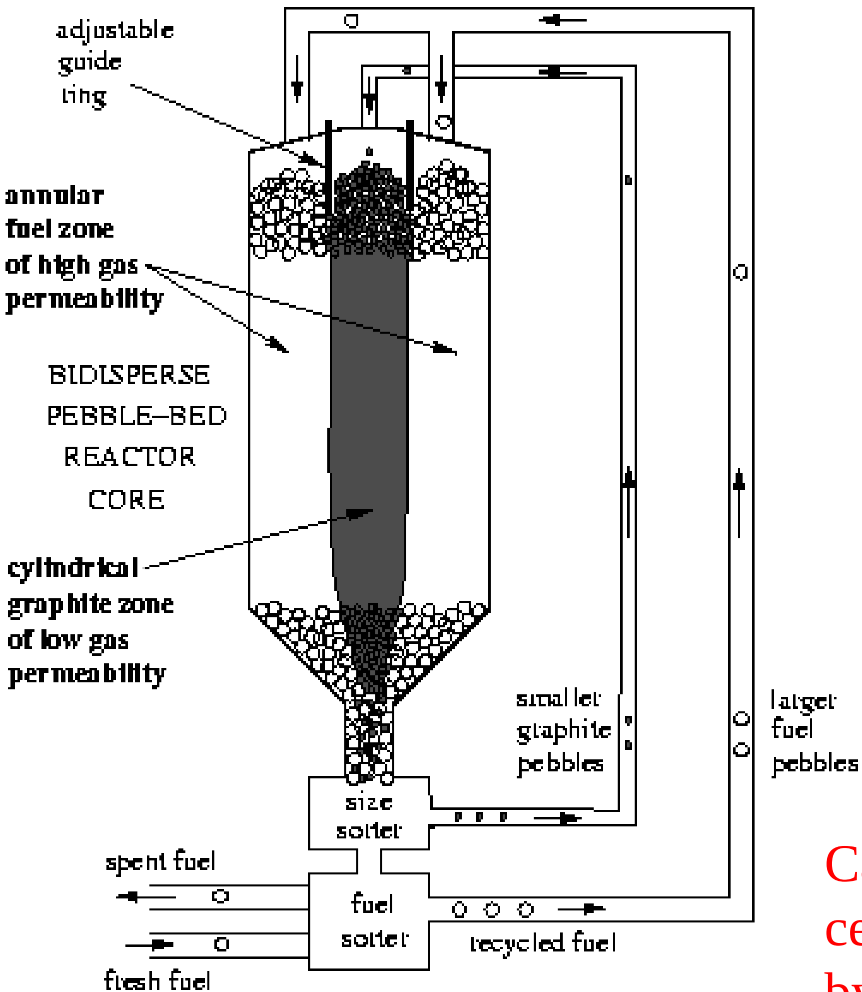
Local Porosity profiles

Blue = 63%, red = 50% volume fraction

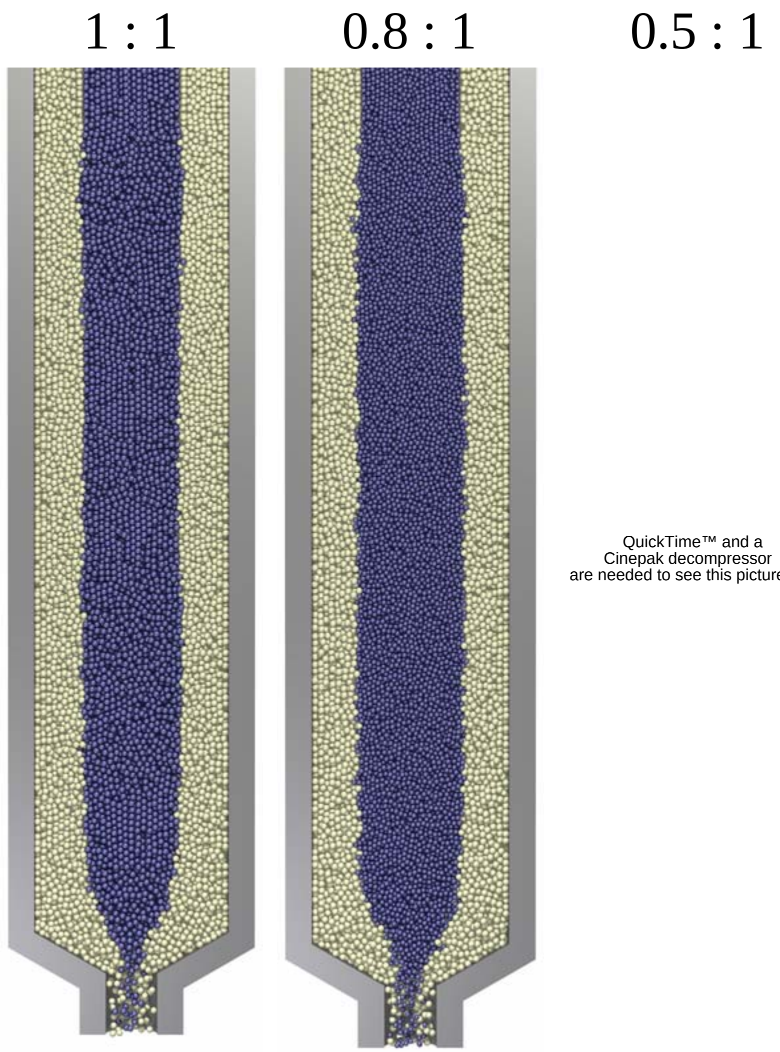


- Upper region: close-packed plug
- Funnel region: 9% lower volume fraction
- 20% lower volume fraction on walls due to local ordering, extends below guide ring
- Nonuniform gas permeability (by <15%)

The Bidisperse PBR Concept



Bazant (2004)



QuickTime™ and a
Cinepak decompressor
are needed to see this picture.

Can reduce gas permeability of the dynamic central column by 75% without any mixing by using 50% smaller moderator pebbles (but 75% smaller causes mixing with fuel)

Conclusions

- *Supercomputing enables full-scale modeling of MPBR pebble flow.* Next step: couple to core neutronics and thermal hydraulics.

- The dynamic central column is stable and does not mix with the fuel.

- The bidisperse concept focuses helium gas flow on the fuel annulus using 50% smaller moderator pebbles in the dynamic column.

- The mean flow is well described by the kinematic model in the funnel, where porosity and gas permeability are 10-15% smaller.

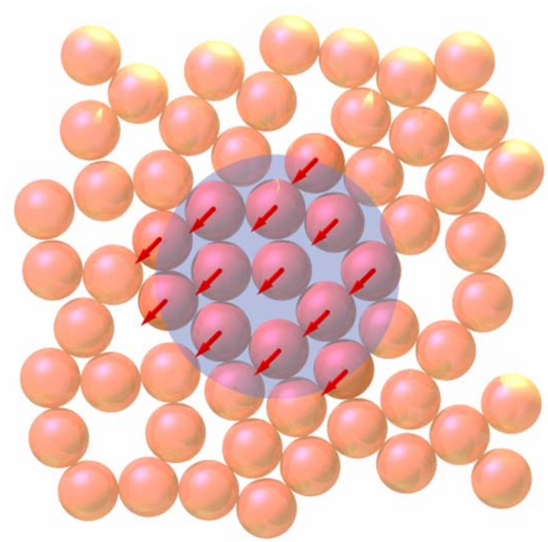
- Ordering occurs near smooth walls and extends below the guide ring.

- We are also developing a fast, multiscale algorithm, based on a new physical mechanism for random-packing dynamics ("spots") …

http://math.mit.edu/dryfluids

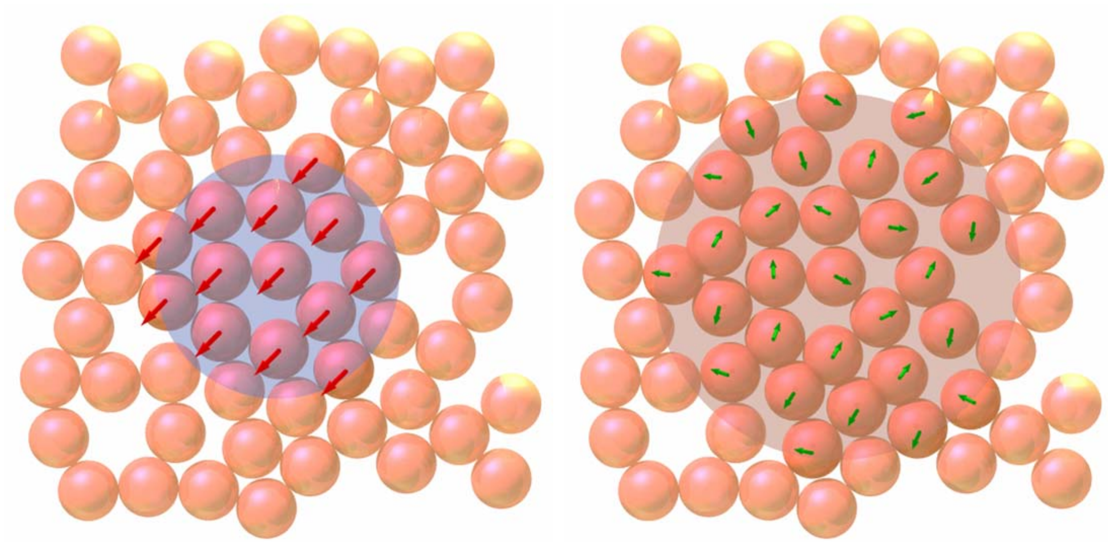
“Multi-scale” Spot Algorithm

1. Basic spot-induced motion



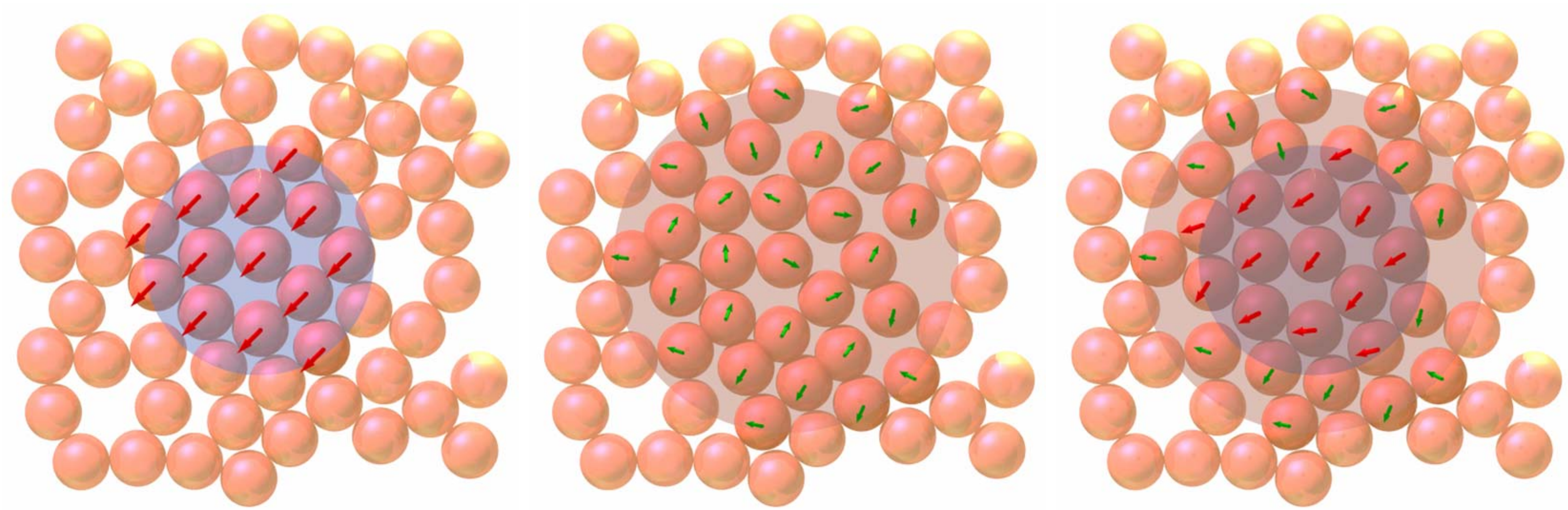
- A “spot” carries a slight excess of interstitial volume, spread over 5 particle diameters
- Spot diffusion due to applied stress (“stochastic plasticity”) causes small block-like displacements of particles

“Multi-scale” Spot Algorithm
2. Relaxation by soft-core repulsion



- Apply a relaxation step to all particles within a larger radius
- All overlapping pairs of particles experience a normal repulsive displacement (soft-core elastic repulsion)
- Very simple model - no “physical” parameters, only *geometry*.

“Multi-scale” Spot Algorithm
3. Net cooperative displacement



- Mean displacements are mostly determined by basic spot motion (80%), but packing constraints are also enforced
- *Can this algorithm preserve reasonable random packings?*
- *Will it preserve the simple analytical features of the model?*

Multiscale Spot Model

In ***Three*** Dimensions

Rycroft, Bazant, Grest, Landry (2005)

Spot Model **DEM**

- Infer 3 spot parameters from DEM, as from expts:

  * radius = 2.6 d

  * volume = 0.33 v

  * diffusion length = 1.39 d

- Relax particles each step with soft-core repulsion

- “Time” = number of drained particles

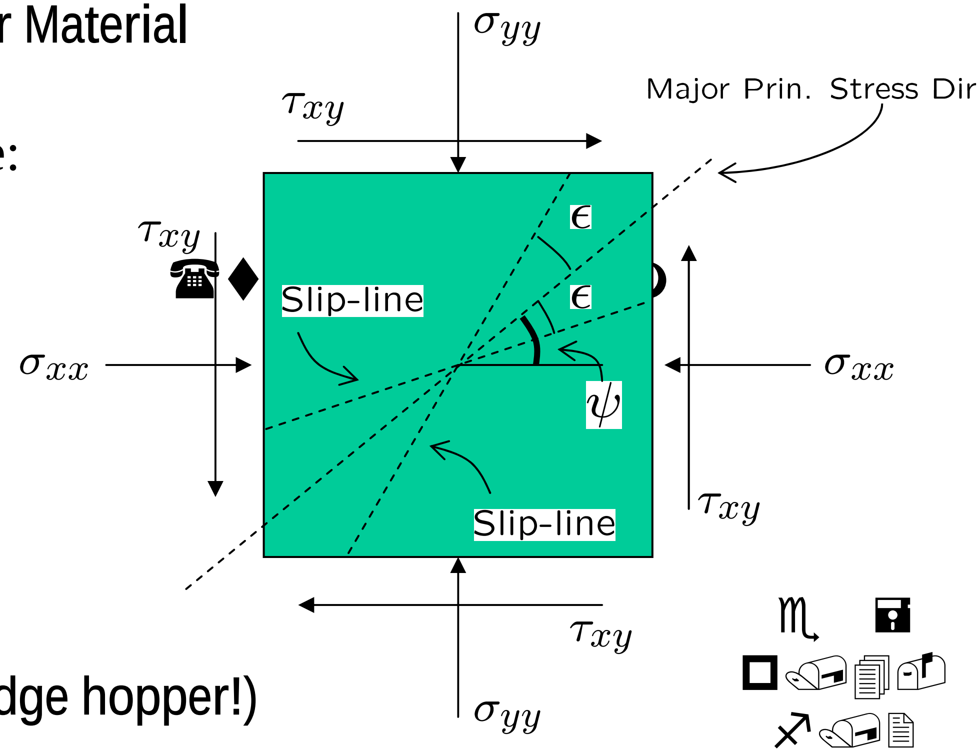
- Very similar results as DEM, but >100x faster!

QuickTime™ and a
Cinepak decompressor
are needed to see this picture.

Classical Mohr-Coulomb Plasticity

1. Theory of Static Stress in a Granular Material

Assume “incipient yield” everywhere:



❍🖫 internal friction coefficient

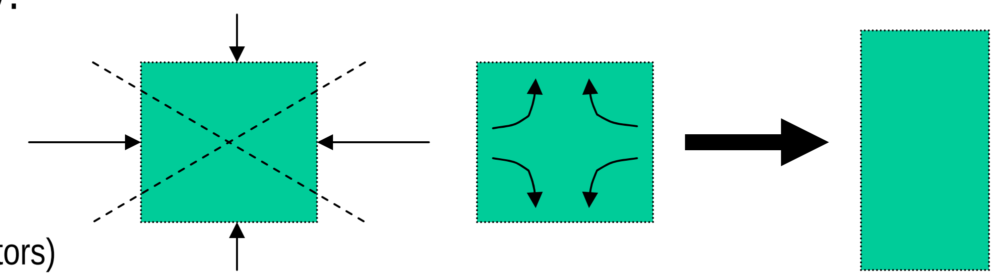
♐= internal failure angle = tan^{-1}❍

2. Theory of Plastic Flow (only in a wedge hopper!)

Levy flow rule / Principle of coaxiality:

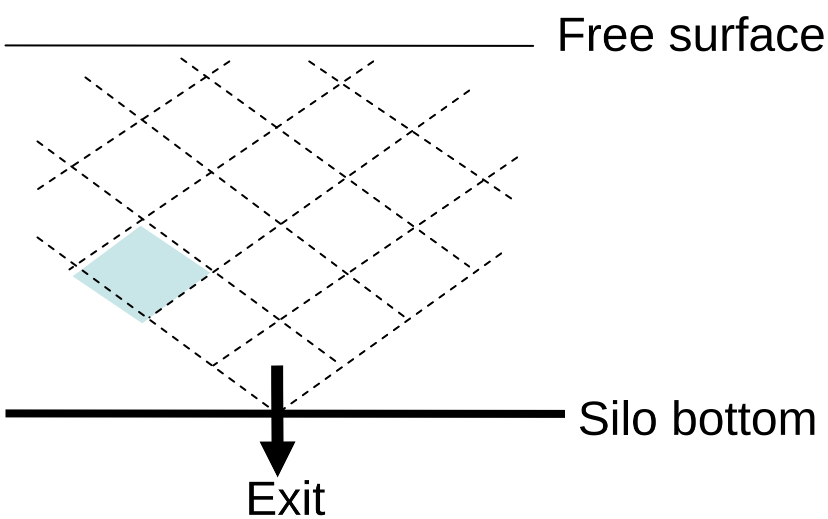
Assume equal, continuous slip
along *both* incipient yield planes

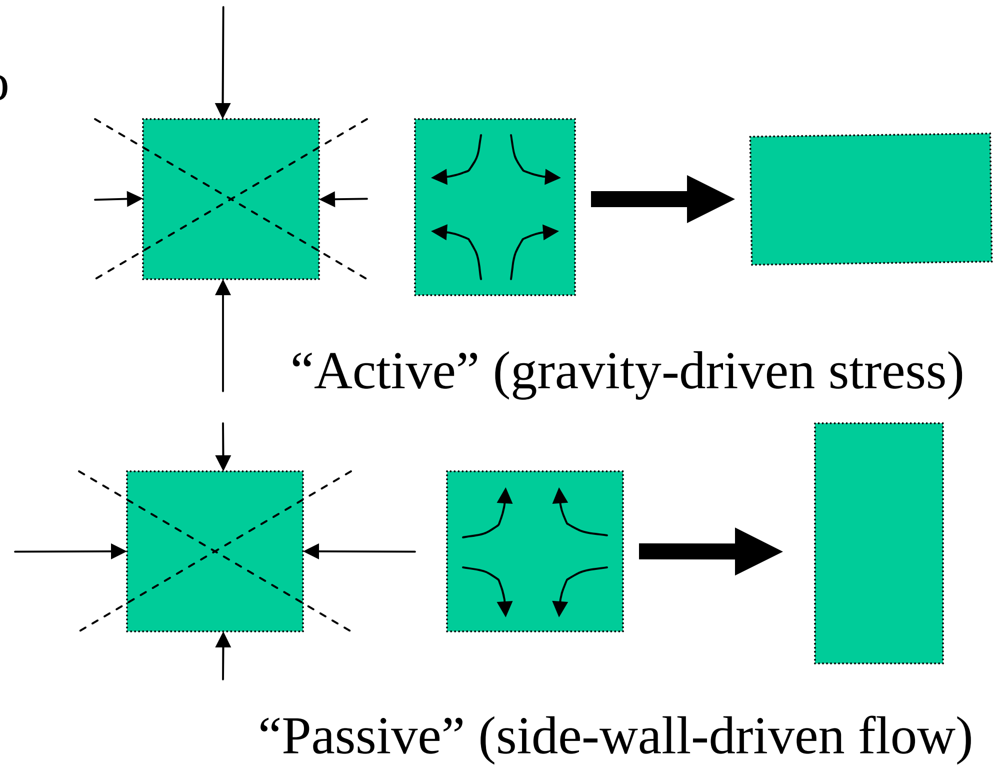
(stress and strain-rate tensors have same eigenvectors)



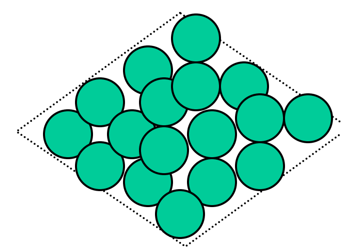
Failures of Classical Mohr-Coulomb Plasticity to Describe Granular Flow

1. Stresses must change from active to passive at the onset of flow in a silo (to preserve coaxiality).

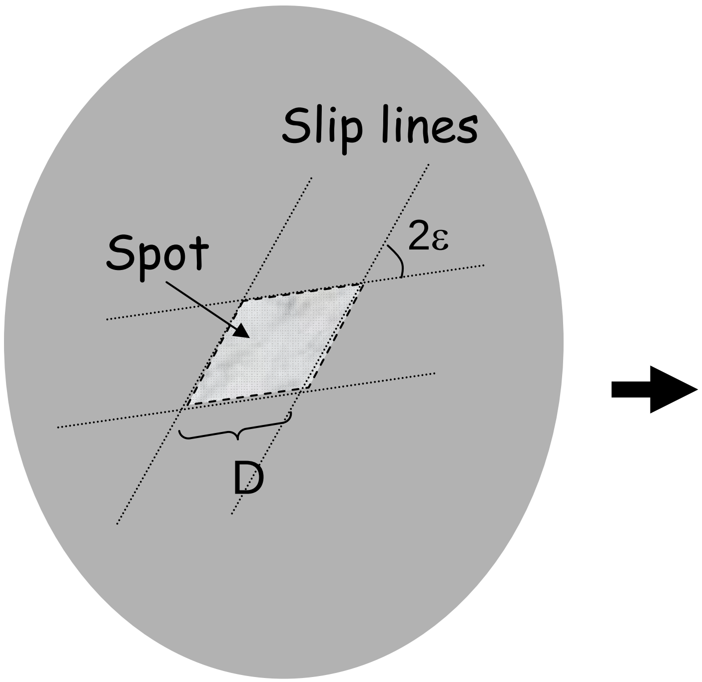


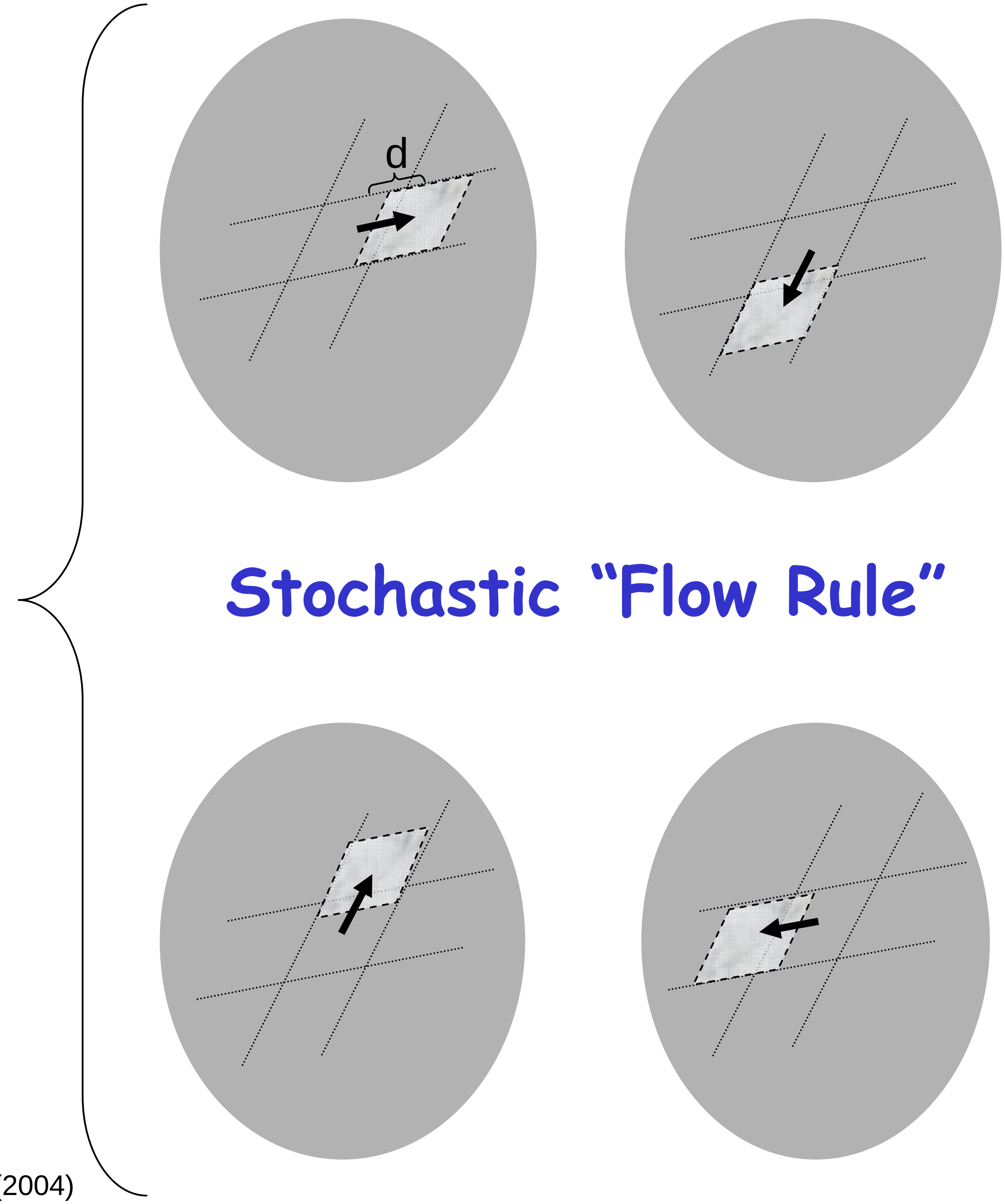


2. Walls produce complicated velocity and stress discontinuities (“shocks”) not seen in experiments with cohesionless grains.
3. No dynamic friction
4. No discreteness and randomness in a “continuum element”



Idea (Ken Kamrin):
Replace coaxiality with
an appropriate discrete
spot mechanism





Stochastic "Flow Rule"

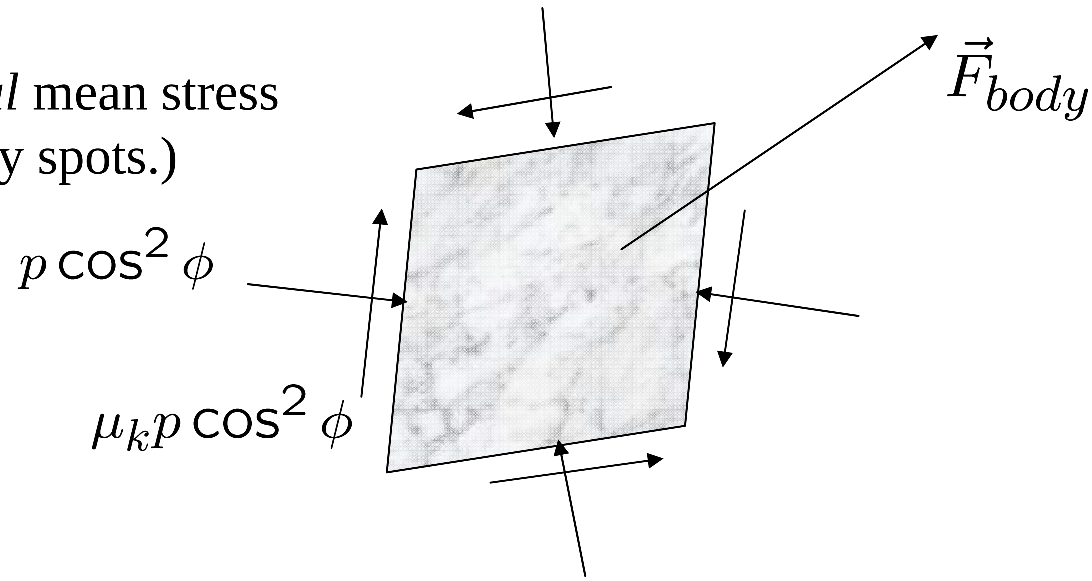
Spots random walk along
Mohr-Coloumb slip lines
(but not on a lattice)

Similar ideas in ***lattice*** models for glasses:
Bulatov and Argon (1993), Garrahan & Chandler (2004)

A Simple Theory of Spot Drift

Spot = localized failure where μ is replaced by μ_k (static to dynamic friction)

(Assume quasi-static *global* mean stress distribution is unaffected by spots.)



Net force on the particles affected by a spot

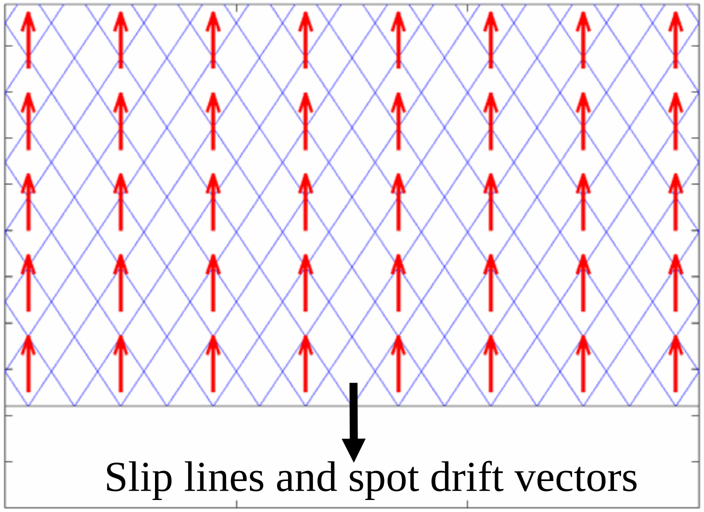
$$\boxed{\vec{F}_{net} = (1 - \mu_k/\mu)\ (\vec{F}_{body} - \cos^2\phi\ \vec{\nabla} p)}$$

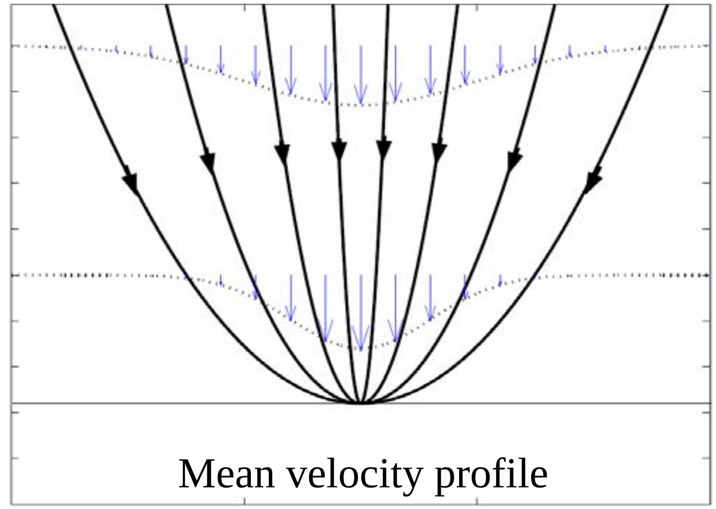
A spot's random walk is biased by this force projected along slip lines.

Use the resulting spot drift and diffusivity in the general theory to obtain the fluid velocity and particle diffusivity…

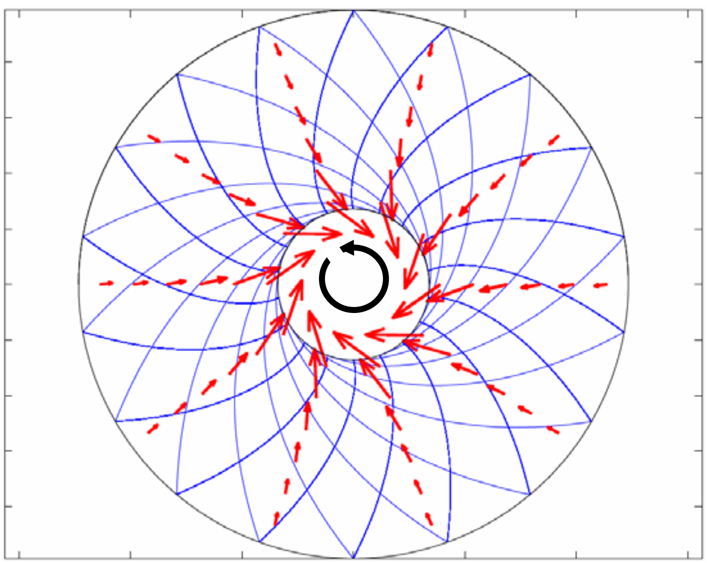
Towards a ***General*** Theory of Dense Granular Flow?

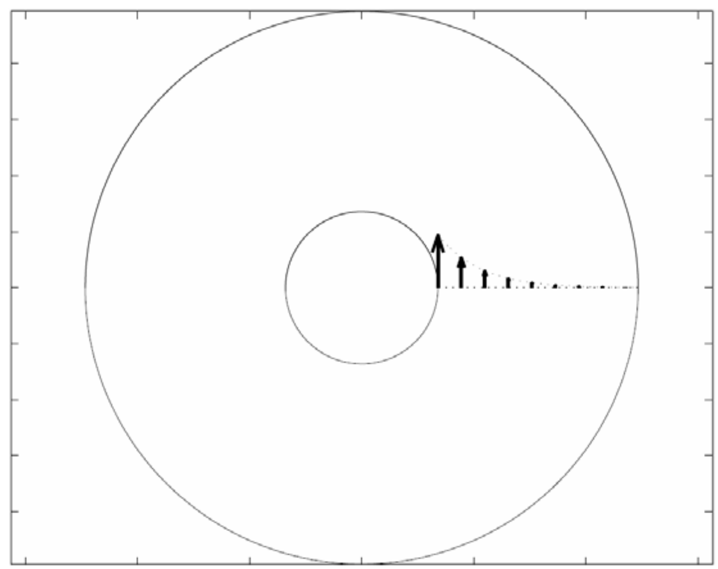
Gravity-driven drainage from a wide quasi-2d silo: Predicts the kinematic model





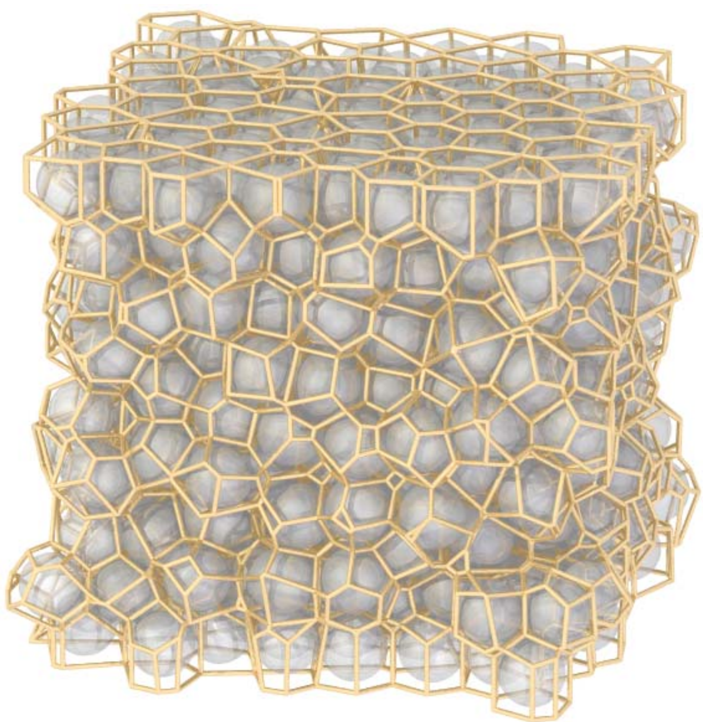
Coette cell with a rotating rough inner wall: Predicts shear localization





Trouble in Paradise?

Spot Model DEM



Particle Voronoi Volumes

Chris Rycroft, PhD thesis

QuickTime™ and a
Cinepak decompressor
are needed to see this picture.

- “Free volume” peaks in regions of highest shear, not the center!
- Maybe somehow alter spot dynamics, or don’t use spots everywhere…

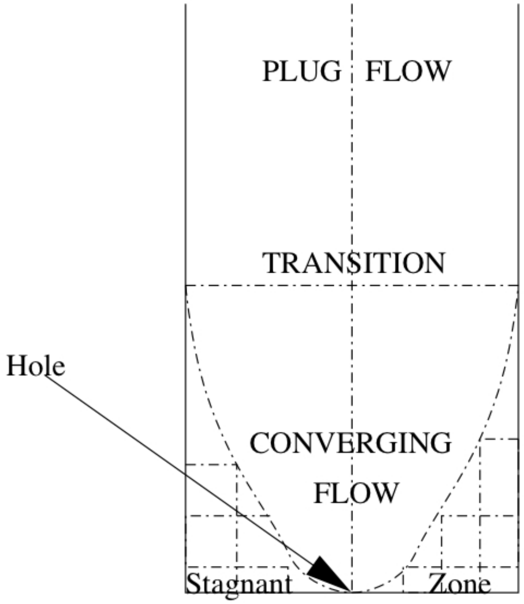
General Theory of Dense Granular Materials: Stochastic ***Elasto***plasticity?

• When forcing is first applied, the granular material responds like an elastic solid.

• Whenever the stability criterion is violated, a plastic “liquid” region at incipient yield is born.

• Stresses in elastic solid and plastic liquid regions evolve under load, separated by free boundaries.

• Solid regions remain stagnant, while liquid regions flow by stochastic plasticity. Microscopic packing dynamics is described by the Spot Model.



Classical engineering picture of silo flow with multiple zones, without any quantitative theory. (Nedderman 1991)

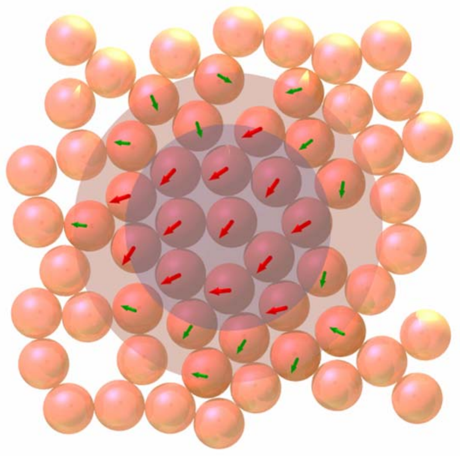
Conclusion

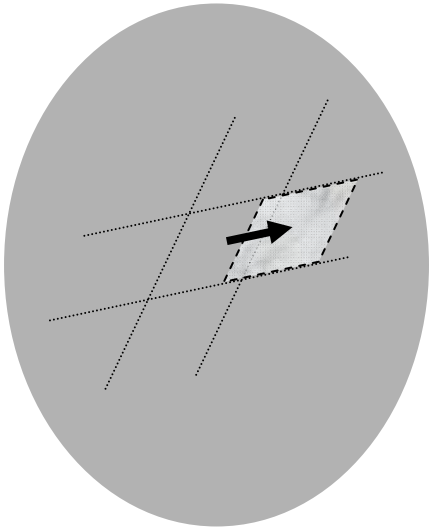
• The Spot Model is a simple, general, and realistic mechanism for the dynamics of dense random packings

• Random walk of spots along slip lines yields a Stochastic Flow Rule for continuum plasticity

• Stochastic Mohr-Coulomb plasticity (+ nonlinear elasticity?) could be a general model for dense granular flow

• Interactions between spots?
Extend to 3d, other materials,…?





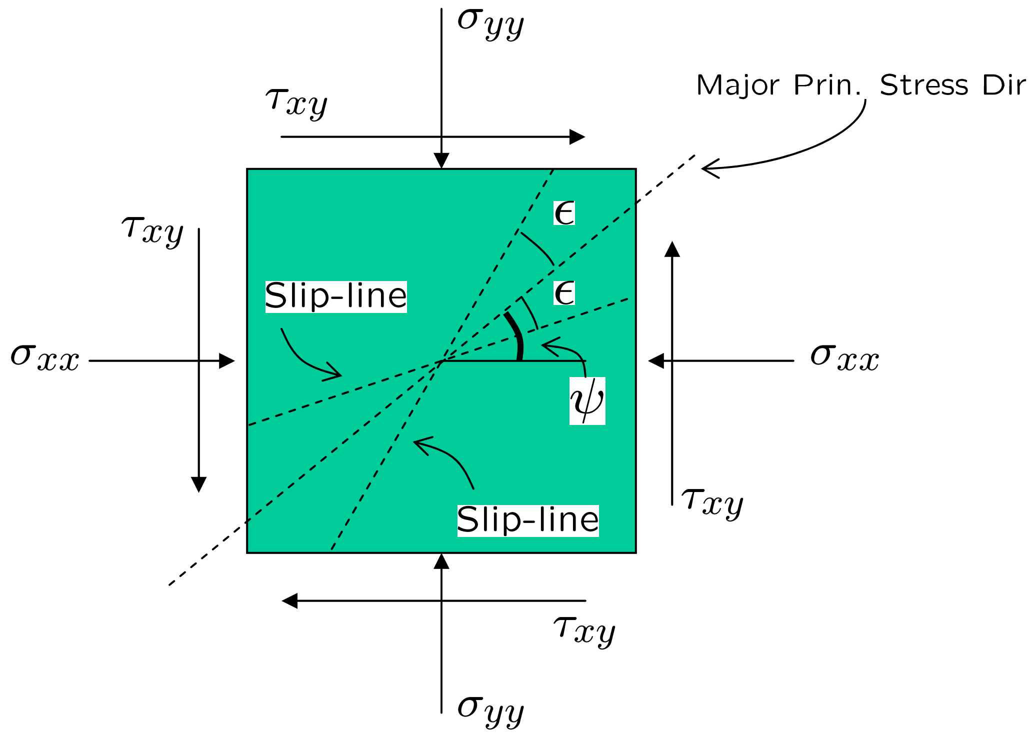
For papers, talks, movies,… **http://math.mit.edu/dryfluids**

Mohr-Coulomb Stress Equations (assuming incipient yield everywhere)

$$\boxed{\begin{aligned}&(1+\sin\phi\cos 2\psi)p_x - 2p\sin\phi\sin 2\psi\ \psi_x + \sin\phi\sin 2\psi\ p_y + 2p\sin\phi\cos 2\psi\ \psi_y = F_x^{body}\\ &\sin\phi\sin 2\psi\ p_x + 2p\sin\phi\cos 2\psi\ \psi_x + (1-\sin\phi\cos 2\psi)p_y + 2p\sin\phi\sin 2\psi\ \psi_y = F_y^{body}\end{aligned}}$$

Characteristics (the slip-lines)

$$\boxed{\begin{aligned}\frac{dy}{dx} &= \tan(\psi-\epsilon)\\ \frac{dy}{dx} &= \tan(\psi+\epsilon)\end{aligned}}$$



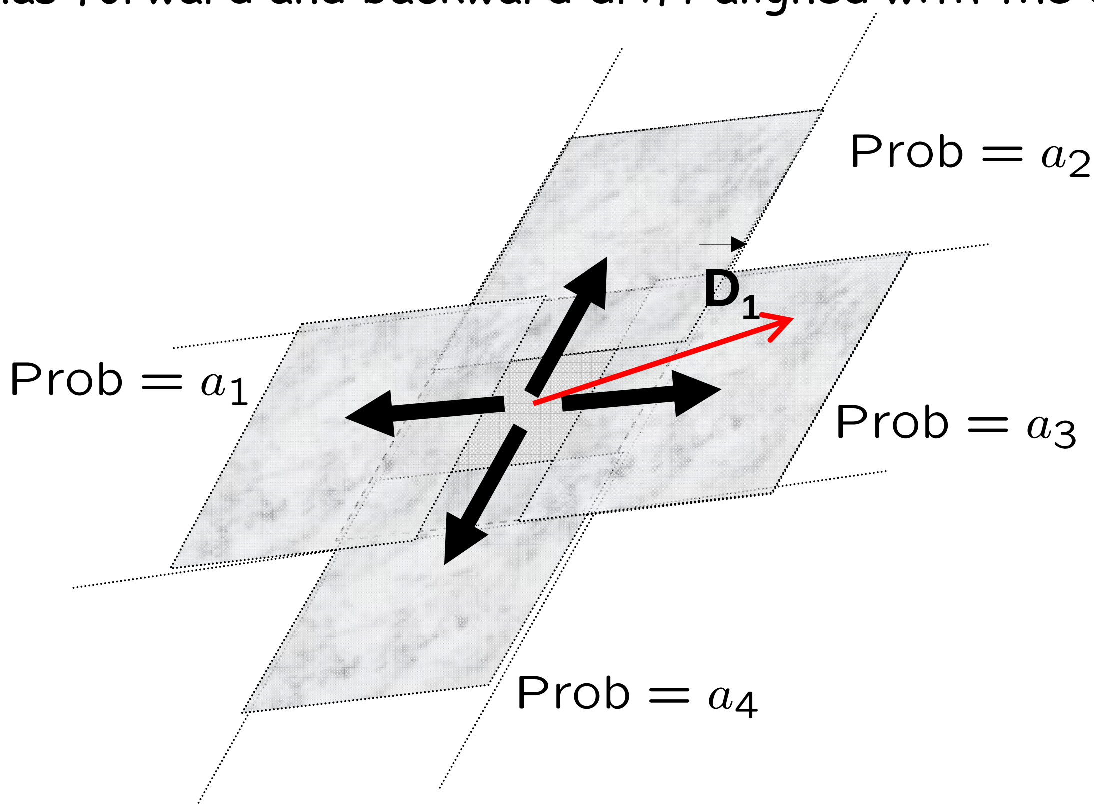
$$p = \frac{\sigma_{xx}+\sigma_{yy}}{2} = \text{Average normal stress}$$

$$\psi = -\frac{1}{2}\arctan\left(\frac{2\tau_{xy}}{\sigma_{xx}-\sigma_{yy}}\right) = \text{Angle anti-clockwise from x-axis to major principal stress direction}$$

- Spot drift opposes the net material force.
- Spots drift through slip-line field constrained only by the geometry of the slip-lines. Probability of motion along a slip-line is proportional to the component of $-F_{net}$ in that direction. Yields drift vector:

$$\vec{D}_1 = -\gamma\,(1-\mu_k/\mu)\left(\mathbf{I} + \cos 2\epsilon \begin{bmatrix} \cos 2\psi & \sin 2\psi \\ \sin 2\psi & -\cos 2\psi \end{bmatrix}\right)(\vec{F}_{body} - \cos^2\phi\,\vec{\nabla} p)$$

- For diffusion coefficient $\underline{D}_2$, must solve for the unique probability distribution over the four possible steps which generates the drift vector and has forward and backward drift aligned with the drift direction.



$$\frac{a_1}{a_4} = \frac{a_3}{a_2}$$